

Inhomogeneous chiral condensates and non-analyticity under an external magnetic field

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We investigate inhomogeneous chiral condensates, such as the so-called dual chiral density wave of dense quark matter, under an external magnetic field at finite real and imaginary chemical potentials. In a model-independent manner, we find that analytic continuation from imaginary to real chemical potential is not possible due to the singularity induced by inhomogeneous chiral condensates at zero chemical potential. From the discussion on the non-analyticity and methods used in lattice QCD simulations, e.g., Taylor expansion, and the analytic continuation with an imaginary chemical potential, it turns out that information on an inhomogeneous chiral condensed phase is missed in the lattice simulations at finite baryon chemical potentials unless the non-analyticity at zero chemical potential is correctly considered. We also discuss an exceptional case without such non-analyticity at zero chemical potential.

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I. INTRODUCTION

Exploring the phase diagram of Quantum Chromodynamics (QCD) is one of the important and interesting subjects in nuclear physics, elementary particle physics, and astrophysics; for a review on the QCD phase diagram see Ref. [1]. *Ab initio* lattice QCD simulations are a powerful and reliable method for analyzing the nonperturbative nature of QCD, but the well-known sign problem arises at finite real chemical potential (μ_R). To circumvent the sign problem, several methods have been proposed so far: the Taylor expansion method, the reweighting method, the canonical approach, and the analytic continuation method from imaginary chemical potentials (μ_I); see for example Ref. [2]. These methods are, however, limited in the $\mu_R/T < 1$ region, where T is the temperature. On the other hand, effective model calculations are useful to investigate the phase diagram at finite T and μ_R , but it is still difficult to quantitatively discuss the phase structure of QCD due to a large ambiguity of the model.

Inhomogeneous chiral condensed phases have been vigorously studied in the QCD phase diagram at finite density within chiral effective models, and also supported from Dyson-Schwinger studies of dense QCD (for a recent review see Ref. [3]), and their stabilities against thermal fluctuations have also been discussed [4, 5]. These phases have the quark condensate taking a spatially inhomogeneous configuration. One example with a one-dimensional modulation includes the so-called dual chiral density wave (DCDW) [6], where the chiral order parameter is spatially modulated with a finite wavenumber (q)

in the single direction. Several studies based on mean-field calculations predict that the inhomogeneous phase can be realized in sufficiently high μ_R region. However, this situation could be changed if we introduce an external magnetic field.

Magnetic aspects of QCD have been attracted much attention in the physics of heavy-ion collision experiments and compact stars (for a review see Ref. [7]). Recently, it has been reported that quark matter with the DCDW condensate could exhibit spontaneous magnetization [8], which may be related to the origin of strong magnetic fields in compact stars. In the presence of the external magnetic field, the most important and interesting point is that the DCDW phase appears even at small values of μ_R except $\mu_R = 0$ within the massless Nambu–Jona-Lasinio (NJL) model [9–11]. This naturally raises the following question: Can we investigate inhomogeneous chiral condensates by using dense lattice QCD simulations at finite μ_R when the DCDW phase appears at very small μ_R ? Here we assume that the inhomogeneous phase can appear in finite and discretized systems.

In this paper, we discuss spatially inhomogeneous chiral condensates and the associated non-analyticity. Then we show the possibility that information on the inhomogeneous phases can be missed in the lattice QCD simulations with the Taylor expansion method and the analytic continuation method from the μ_I region to the μ_R region. We call this problem the “information missing problem.” We find that the applicable range of μ_R in the dense lattice QCD simulations at finite μ_R is strongly restricted, and such numerical simulations cannot describe the correct system with inhomogeneous chiral condensates if we neglect the non-analytic properties at $\mu^2 = 0$. Some problems in the canonical and reweighting methods are also discussed. In addition, an exceptional case where there is no non-analyticity at $\mu^2 = 0$ is presented. Here we note that the same problem would exist in zero magnetic field, because the DCDW phase can appear also in the case without the external magnetic field.

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II. INHOMOGENEOUS CHIRAL CONDENSATES AT IMAGINARY CHEMICAL POTENTIAL

In realistic systems, the grand canonical partition function (Z) must be real. It is also valid in the presence of inhomogeneous chiral condensates under a constant magnetic field, since the ground states of inhomogeneous phases correspond to solutions of Hamiltonian with μ_R , i.e., $Z(T, \mu_R, B; q) \in \mathbb{R}$, where B is the strength of the external magnetic field. This relation is simply manifested in the NJL model. The same discussion in the Polyakov-loop-extended NJL model requires some extensions of the formalism, e.g., considering a complex path contour [12–14] due to the model sign problem.

Here we only focus on the DCDW phase, since it is well known that the so-called real kink crystal (RKC) phase does not appear in the μ_I region at least in the Gross-Neveu model [15]. Also, the RKC phase shows no significant dependence on the external magnetic field and thus appears at sufficiently high μ_R , while the DCDW phase is extended to small μ_R region. Therefore, we do not here treat the RKC condensate, since we are interested in the inhomogeneous phase at small μ_R .

Assuming that the DCDW type inhomogeneous condensation arises in the presence of the uniform magnetic field, the massless NJL Lagrangian density with the mean-field approximation takes the form [9]

$$\mathcal{L} = \bar{\psi} \left(i\gamma^\mu D_\mu + \mu\gamma^0 - m + \gamma^5 \gamma^3 \frac{q}{2} \right) \psi - \frac{m^2}{4G}, \quad (1)$$

where ψ is the quark field, γ^μ are Dirac matrices, μ is the quark chemical potential, G is the coupling constant, the constituent quark mass $m = -2G\Delta$ with Δ the constant amplitude of the DCDW, and the covariant derivative $D_\mu = \partial_\mu - ieA_\mu$ with e the electric charge and A_μ the external magnetic field. Here A_μ is directed along the z axis, $\nabla \times \mathbf{A} = B\hat{z}$. The Lagrangian density given above is the one-flavor case but can be easily extended to the two-flavor one by considering the π^0 -modulation. Then the quark determinant in the partition function takes the form

$$\ln Z \sim \text{Tr} \ln (i\gamma^\mu D_\mu + \mu\gamma^0 - m + \gamma^5 \gamma^3 q/2). \quad (2)$$

Here we can show the symmetry of the system model-independently, while the analysis described above is model dependent. To this end, we evaluate Z by a Ginzburg-Landau (GL) expansion.

In general, q -odd terms are not banned in the expansion of Z with respect to q under the constant magnetic field:

$$Z = \alpha_0 + \alpha_1 q + \alpha_2 q^2 + \alpha_3 q^3 + \alpha_4 q^4 + \dots, \quad (3)$$

where α_n ($n = 0, 1, 2, \dots$) are expansion coefficients determined by effective chiral models like the NJL model. Here the q -odd terms can be induced by a scalar quantity

$(\mathbf{q} \cdot \mathbf{B})$ without violating the rotational invariance. The coefficients α_{2n} (α_{2n+1}) should be an even (odd) function of B and μ , respectively, which can be understood by taking the trace of Dirac space in Eq. (2). This implies that q of the DCDW can take an imaginary value in the finite μ_I region so as to manifest the reality of Z , i.e., $Z(T, \mu_I, B; q = iq_I) \in \mathbb{R}$ where $q_I \in \mathbb{R}$. This situation can arise in the case where an anomalous quark number density is proportional to q [10], since the quark number density (n_q) should be pure imaginary in the μ_I region and q acts as n_q . A similar situation can also be expected, e.g., in complex chemical potential system, where Z should be a complex value.

By summarizing the above discussions, we can reach the following scenarios:

Scenario A — The DCDW phase does not appear at finite μ_I .

Scenario B — The DCDW phase appears at finite μ_I , but the partition function becomes complex.

Scenario C — The DCDW phase appears at finite μ_I , and the partition function is real.

Each scenario is illustrated in Fig. 1. At a point very close to $\mu^2 = 0$, it is enough to regard Z as only the first few terms in Eq. (3), since we can consider that q becomes quite small if there is no first-order transition at $\mu^2 = 0$. In the region of $\mu^2 > 0$, the stationary condition for q , $\partial Z / \partial q = 0$, yields $q = -\alpha_1 / 2\alpha_2 \sim \mu$. Therefore, q^2 is described as a linear function of μ^2 , as shown in Fig. 1. Here one can model-independently consider that Z contains α_1 , since it is known in Ref. [10] that the GL coefficient α_1 evaluated within the NJL model contains the Wess-Zumino-Witten (WZW) term [16] derived from chiral anomaly. In Scenario B, the wave number is real at finite μ_I , $q \in \mathbb{R}$, while in Scenario C it becomes pure imaginary, $iq \in \mathbb{R}$. Although we need a model calculation to see which of scenarios is realized, our purpose in this paper is to qualitatively understand inhomogeneous chiral condensates and their associated non-analyticities, so that we leave it for future work. In the following, we discuss details of each scenario without model assumptions.

A. Non-analyticity and analytic continuation

We discuss the analytic continuation from the μ_I to the μ_R region on the μ^2 axis. Here we introduce two holomorphic functions, F_1 and F_2 , which describe regions $C_1 = \{\mu^2 \in \mathbb{R} \mid 0 < (\mu/T)^2 < \epsilon\}$ and $C_2 = \{\mu^2 \in \mathbb{R} \mid -\epsilon < (\mu/T)^2 < 0\}$, where ϵ is a positive infinitesimal value. If F_1 and F_2 have the connected domain at $\mu^2 = 0$, we can use the analytic continuation exactly. In Scenarios A and B, there exists the singularity at $\mu^2 = 0$ and hence the analytic continuation is no longer possible due to $F_1 \neq F_2$ for inhomogeneous chiral condensates. In Scenario C, on

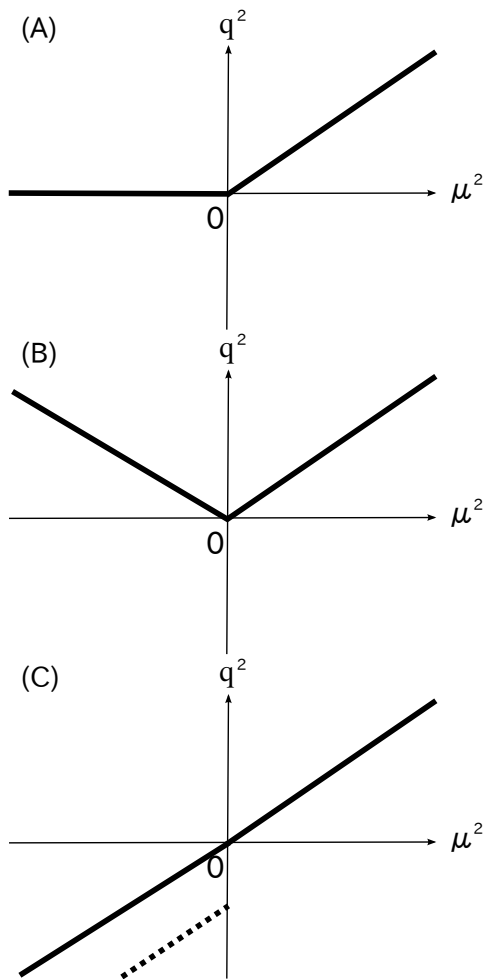


FIG. 1: Schematic figures with respect to q^2 as a function of μ^2 at very close to $\mu^2 = 0$ for each scenario. The $\mu^2 = 0$ point becomes singular, except the solid lined case in Scenario C.

the other hand, there is a possibility that the analytic continuation still works.

1. Scenarios A and B

In Scenario A, the $\mu^2 = 0$ line becomes singular, so that the analytic continuation is impossible. This situation, however, becomes non-trivial when a Taylor expansion in terms of μ_R at $\mu^2 = 0$ is considered. The Taylor series cannot reproduce the non-analyticity and hence can describe only one side of the solution. To choose which solution is realized (whether the homogeneous or inhomogeneous solutions), we need a restriction to the Taylor series, since we cannot mathematically determine the Taylor series just on such a singular point. In Scenario B, the situation is completely the same as Scenario A, where the $\mu^2 = 0$ line is the singular line due to $\text{Im } Z \neq 0$ at finite μ_I . The Taylor series with the restriction, $\text{Im } Z = 0$, may lead to solutions continued to

the μ_R region. However, such a series is not mathematically well-defined. We note here that one can consider a first-order transition at $\mu^2 = 0$, where q^2 has a finite positive value in the $\mu^2 \rightarrow -0$ limit, but our conclusion is not changed in this scenario.

2. Scenario C

In Scenario C, the wavenumber has a nonzero real value, $q_R \neq 0$, in the C_1 region, while in the C_2 region it becomes pure imaginary, $q_I \neq 0$. Here Z has only the q -even terms at $\mu^2 = 0$, since α_{2n+1} is the odd function of μ in the expansion (3). Now we can further consider two situations, (I) and (II):

Scenario C(I) — Assuming that q vanishes in the $\mu^2 \rightarrow +0$ limit, $\alpha_2(T, \mu)$ should be positive at $\mu = 0$. In the $\mu^2 \rightarrow -0$ limit, on the other hand, the coefficient of q_I^2 should be $-\alpha_2 < 0$ for $q = iq_I$. Thus, the point, $q_I = 0$, cannot be a minimum of Z , and q_I does not vanish in the $\mu^2 \rightarrow -0$ limit. In this case, there is the first-order phase transition at $\mu^2 = 0$. However, there is no reason that the translational (rotational) symmetry is spontaneously broken in the $\mu^2 \rightarrow -0$ limit as well.

Scenario C(II) — In Scenario C(I) it is assumed that $\alpha_2(T, \mu = 0) \neq 0$, but $\alpha_2 = 0$ can be acceptable. In this case, it seems possible to perform the analytic continuation because q^2 in the $\mu^2 \rightarrow \pm 0$ limit can be smooth at $\mu^2 = 0$. This situation is quite similar to the quark number density, n_q , in the system with $B = 0$, since n_q^2 is positive (negative) at finite μ_R (μ_I) and n_q^2 is smoothly connected at $\mu^2 = 0$ when we take the $\mu^2 \rightarrow \pm 0$ limit.

In Scenario C(I), the analytic continuation is impossible due to the first-order transition at $\mu^2 = 0$. Although the Taylor series constructed just on the singular point is not mathematically well-defined, each solution of inhomogeneous condensates may be reproduced under a suitable choice of input configurations. However, this situation is not realistic, since there is no reason to consider that the spontaneous translational (rotational) symmetry breaking occurs at $\mu^2 = 0$. Thus, we can exclude this situation. In Scenario C(II), on the other hand, there has the possibility that the analytic continuation works because q^2 becomes smooth at $\mu^2 = 0$ as same as n_q^2 in the system with vanishing B . Only this scenario has the well-defined analytic continuation process and the Taylor series constructed at $\mu^2 = 0$.

If inhomogeneous chiral condensates appear on the QCD phase diagram, the singular line, $\mu^2 = 0$, should be exist. Note that this singular line can appear at smaller μ_R/T than the natural boundary of the Taylor series in the absence of the magnetic field or the existence of the nonzero current mass. To avoid such a singularity in the analytic continuation, we can consider the complex

chemical potential. However, lattice QCD simulations and effective model calculations are quite difficult, since the singular region should have nonzero $\text{Im } Z$.

B. Non-analyticity and dense lattice QCD simulations

Now we discuss the consequences of the non-analyticity for several methods to work around the sign problem used in the lattice QCD simulations at finite chemical potentials.

The trivial case is the analytic continuation method from μ_I to μ_R [17–21]. This is nothing but our discussion about the analytic continuation. Thus, it is not feasible.

The reweighting method [22–25] can go beyond the non-analytic point in principle. However, the overlap problem is important in this method. The μ_I region cannot be used for the creation of the probability in the important sampling procedure, since in Scenario A the overlap which can induce $q \neq 0$ should be vanished or very small, and there is the sign problem at finite μ_I in Scenario B. Also, the $\mu^2 = 0$ point may have a small overlap problem. If we know regions where the sign problem does not arise and inhomogeneous chiral condensates exist, the reweighting method should completely work, while we do not know such a convenient region at present.

The canonical approach [26–30] is based on the fact that the grand canonical partition function with μ_R can be constructed from the one with μ_I , which is valid if the quark number density is a good quantum number. In this method, we do not directly use the analytic continuation, so that the non-analyticity does not affect this method in principle. However, it is quite difficult to pick up information on inhomogeneous chiral condensates, since some inhomogeneous properties should be hidden when we calculate the grand canonical partition function or some observables via the canonical partition function. This fact should be consistent with the results of a Lee-Yang zero analysis in QCD [31–33], since we only see the distribution of zeros and hence it is difficult to clarify the existence of inhomogeneous phases even if we can find any phase transitions from the behavior of zeros.

On the other hand, the Taylor expansion method [34, 35] is nontrivial. Since this method is deeply related to the analytic continuation method, the Taylor series plays a crucial role. The Taylor series in the Taylor expansion method constructed at $\mu^2 = 0$ is the holomorphic function. Thus, the μ_R and μ_I regions cannot be simultaneously reproduced because there is the non-analyticity at $\mu^2 = 0$. Mathematically, such Taylor series are not well-defined, but one can describe the both-side of solutions by considering the restriction to make the Taylor series describing the desirable limit by hand in the numerical calculations. This procedure may be affected by the numerical error.

From the above discussion, we find that since the $\mu^2 = 0$ point becomes the singular point, extreme care

should be taken to perform the lattice QCD simulations with the Taylor expansion method, the reweighting method, the canonical approach, and the analytic continuation method in the presence of the magnetic field. If the effect of the non-analyticity at $\mu^2 = 0$ are not correctly treated, information about the inhomogeneous chiral condensates should be missed in the Taylor expansion and analytic continuation methods. Such a non-analyticity can be taken into account by imposing the restriction mentioned above. Therefore, the information missing problem should be carefully considered in the dense lattice QCD simulations.

The information missing problem can be avoided in the complex Langevin method [36, 37] and the Lefschetz-thimble path integral method [38–40], since the dense lattice QCD simulation can be directly performed at finite μ_R . However, both methods are far from perfection: there is no guarantee that the complex Langevin method leads to the correct answer when logarithmic terms exist in the action (see, e.g., Refs [41–43], and Ref. [44] from the viewpoint of the singular drift term). The Lefschetz-thimble path integral method can provide the correct answer in principle, but the actual lattice calculation method is not completed, e.g., how to include the multi-thimble contributions.

The effective model approaches, on the other hand, are free from the information missing problem. The lattice QCD simulations without the assumption of inhomogeneous chiral condensates can be possible by the suitable choice of spatial boundary conditions. If the effective models are constrained by such lattice QCD data at finite μ_I , one can obtain the reliable model for the system without inhomogeneous phases. This method is nothing but the imaginary chemical potential matching approach [45, 46]. However, information about inhomogeneous chiral condensed phases can be introduced to the effective models by assuming the shape of the solution. This is a standard procedure to include the inhomogeneous condensates in the effective model approach. By unifying the substitution procedure and the imaginary chemical potential matching approach, one can investigate *full QCD*.

III. SUMMARY

In this paper, we have investigated the properties of inhomogeneous chiral condensates at finite imaginary chemical potential in the presence of an external magnetic field. From the reality of the partition function and the symmetry argument, we have considered two possible scenarios for the DCDW at finite μ_I . In both scenarios, the $\mu^2 = 0$ point becomes the singular, which is induced by the inhomogeneous condensates. This singularity disturbs the investigation of inhomogeneous chiral condensates, and hence information of such condensates sometimes is missed, i.e., the information missing problem. We found that the information missing problem can

appear in the lattice QCD simulation with the Taylor expansion and analytic continuation methods. Problems to observe the inhomogeneous chiral condensates by using the reweighting method and the canonical approach are also discussed. Moreover, we considered the exceptional case where q^2 becomes negative.

In the analytic continuation, holomorphic functions, e.g., the Taylor series, play a crucial role. If the $\mu^2 = 0$ point becomes the connected domain where two holomorphic functions prepared in the μ_R and μ_I regions coincide, the present information missing problem does not arise. However, there exists the singularity at $\mu^2 = 0$, which is induced from the different form of chiral condensates or the imaginary part of the partition function. Thus, the analytic continuation from the $\mu^2 \leq 0$ region is not possible, since the line $\mu^2 = 0$ forms the singular line. This fact leads to that the Taylor expansion method require an extreme care if the Taylor series is constructed at $\mu^2 = 0$, the singular point. To correctly construct the Taylor series which continues to the μ_R region, some restrictions are required in the numerical code. It should be noted that we can still consider Scenario C(II) which has the well-defined analytic continuation. However, even if which scenarios are realized, we must check the behavior of q^2 at $\mu^2 < 0$ before investigating the $\mu^2 > 0$ region to clarify the existence of non-analyticity.

For finite current quark masses, the singular line can be sifted at finite μ_R region, which leads to the possibility that the singular line appears at the smaller μ_R/T than the natural boundary of the Taylor series. In this case, the information missing problem becomes more serious. Consequently, the applicable range of the Taylor expansion method and that of the analytic continua-

tion method are strongly restricted. It should be noted that we cannot estimate the position of the singular line by only using the lattice QCD data, unlike the natural boundary which can be estimated from the convergence behavior of the series. Meanwhile, a nonzero current quark mass gives rise to the configuration change of the DCDW condensate [47].

Possible promising methods to overcome the information missing problem at large μ_R would include the unification of the imaginary chemical potential matching approach and the inputting of the solutions of inhomogeneous chiral condensates. In this case, one can obtain reliable effective models at finite μ_R without the inhomogeneous phases, but the information on the inhomogeneous condensations can be restored by inputting the solution. In this method, the lattice QCD data without inhomogeneous chiral condensates at finite μ_I is required but can be obtained if the spatial boundary conditions are suitably imposed. Therefore, we do not need details of information about the inhomogeneous condensates at finite μ_I . Also, it is interesting to combine this approach with a nonperturbative method, e.g., the functional renormalization group method or the Dyson-Schwinger formalism. These topics will be considered in future studies.

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